UNPUBLISHED PRELIMINARY DATA

FIRST QUARTERLY STATUS REPORT
Request No. R-05-030-001
for the period 1 February-30 April 1965

During the first quarter of the contract period, work was done on the problems III 1 - 2, III 4 - 6 of the contract proposal, and some work necessary for III 3, III 7. The state of progress in the solution of the different specific problems is as follows:

III 1, 2. Quantitative calculations of the interfacial energy and the nucleation probability.

All analytical work except that to be done by IBM - Formac has been completed. This involves (1) the formulas for the interfacial energy as function of the size and shape of the crystal, its orientation, its misfit and elastic parameters, (2) the equations for the equilibrium form of the crystal as function of the parameters mentioned above and as function of the surface energy of nucleating crystal and substrate, (3) the Gibbs free energy of the equilibrium form and its second derivative as function of the parameters mentioned above, and (4) the number of atoms per nucleus as function of super-saturation. Programming of the formulas is presently being started.

III 3. Comparison of theory and experiment.

It has been found recently that the epitaxy of f.c.c. metals on NaCl depends strongly upon the history of the NaCl surface and the vacuum conditions during deposition. In order to make a meaningful comparison with theory which does not directly provide for such a dependence, it is necessary to obtain an understanding of this dependence. With this goal in mind, epitaxy experiments with Au on

NaCl were performed in an ultra-high vacuum electron diffraction system with a base pressure of 2×10^{-10} torr. The results to date suggest two possible causes for the influence of the history of the surface and of the vacuum conditions on epitaxy: either the secondary agglomeration process or the nucleation process along steps is influenced. More experiments, now underway, are needed to decide between these two possibilities.

III. 4. Pyrolytic epitaxy of graphite on crystals with fluorite structure.

Considerable difficulty is being encountered in reproducing the formation of epitaxial graphite on CaF_2 and BaF_2 by decomposition of CH_4 at temperatures between 800°C and 1100°C and pressures from 5×10^{-4} to 1×10^{-3} torr, both in a metal and a glass system. The cause for this lack of reproducibility is presently not known, the experiments are continuing.

III 5. Influence of radiation damage on epitaxy on compound crystals.

During the variation of the parameters involved (substrate temperature, electron beam current density, irradiation time, recovering time, evaporation rate, residual gas) a striking dependence of the nucleation process upon residual gas was discovered. All attention since has been directed towards the influence of the gas on the nucleation. It was found that in the presence of He, H_2 and N_2, NaCl grows on NaCl cleavage planes by simply continuing the crystal, while in the presence of CO, CO_2, H_2O and C_2H_2 during irradiation nuclei in a different orientation ($\{110\}_{nucleus}$ //

$\{100\}_{base}$, $\langle 001\rangle_{nucleus}$ // $\langle 110\rangle_{base}$) are formed. The experiments are continuing.

III 6. The monolayer growth of metals.

The early states of growth of Ag and Au on a {110} plane of W was studied both in an ultra high vacuum electron diffraction system and in a low energy electron diffraction system. The preliminary results indicate that the initial layer has a very low degree of order on a clean surface, while on a surface covered with a chemisorted gas layer oriented crystallites are already formed initially. In the films more than a monolayer thick three-dimensional epitaxial crystals with the {111} plane parallel to the substrate are formed. Desorption experiments indicate that the bond between Ag and Au atoms of the first monolayer and the substrate is not much stronger than between Ag and Cu atoms respectively.

III 7. Alkali and alkaline earth films on W and Mo

Preliminary studies have been made to provide well defined {110} surfaces of W crystals for these experiments. This involved proper pretreatment of the crystals to free them from disturbing impurities in the bulk and at the surface and to form well defined adsorption layers, mainly of O_2 and CO.